Can You Breathe in Space?

Searching for Molecular Oxygen in the Interstellar Medium

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“Oxygen in Space”

Cergy-Pointoise, France

16 October 2018

Portrait of Antoine-Laurent Lavoisier and his wife by Jacques-Louis David, ca. 1788

Early History of Molecular Oxygen

Joseph Priestly (1774) and Carl Scheele (1772) produced O_2 by heating MgO

Called “dephlogistonated air” and “fire air”

The name “Oxygen” was coined by Antoine Lavoisier* in 1777

Lavoisier recognized many important aspects of oxygen including ability to form acids, which led to the name, which comes from Greek words for “acid former”

Allotropic forms of oxygen include $\mathbf{O_2}$ {molecular oxygen) and $\mathbf{O_3}$ (ozone)

* Lavoisier was executed by guillotine in 1794 but 2 years later was exonerated and confiscated property was returned to his widow

A Prescient Paper – Mentioning CO, CS, HCN, H_2O, and NH_3 as "of interest to radio astronomy"

1957 International Astronomical Union Symposium 4, 92

PAPER 16

MICROWAVE AND RADIO-FREQUENCY RESONANCE LINES OF INTEREST TO RADIO ASTRONOMY

C. H. TOWNES

Physical Laboratory, Ecole Normale Supérieure, Paris

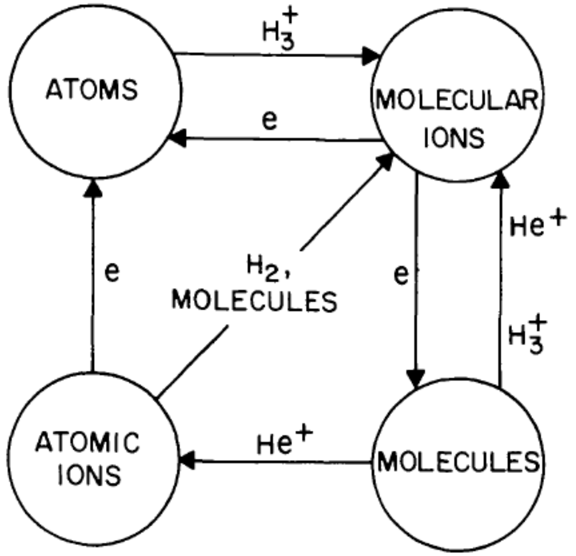
And now the very last sentence:

Additional absorption or emission lines due to gases in the earth's atmosphere are probably immediately detectable; the most obvious of these cases is the rich microwave spectrum of O_2.

O_2 was measured in Earth's atmosphere by microwave absorption in 1972 (or before). But what about interstellar space? Why should we care about this molecule in particular?

Gas-Phase Chemistry of O_2 in the ISM

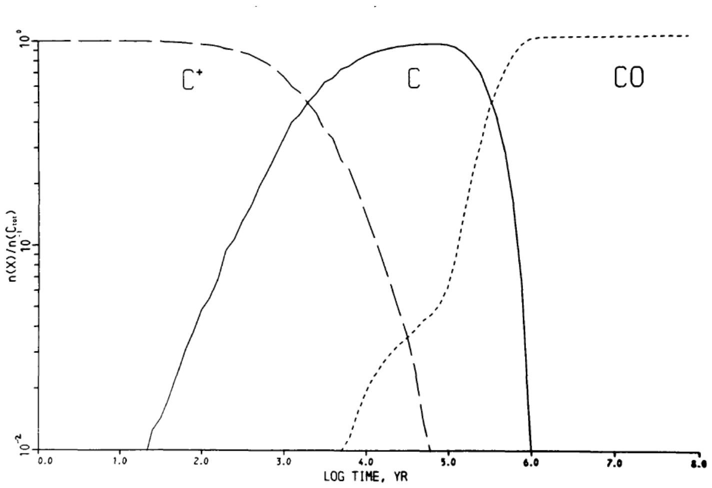
- Herbst & Klemperer (1973) and Watson (1973) developed models for interstellar chemistry based heavily on ion molecule reactions (which lack activation barriers)
- Steady-state calculations with CR ionization rate and H^2 density as free parameters
- $X(O_2) = 2x10^{-6}$ for $n(H_2) = 10^4\ cm^{-3}$ and lower at higher densities. Only a small fraction of available oxygen is in the form of O_2 (H&K)



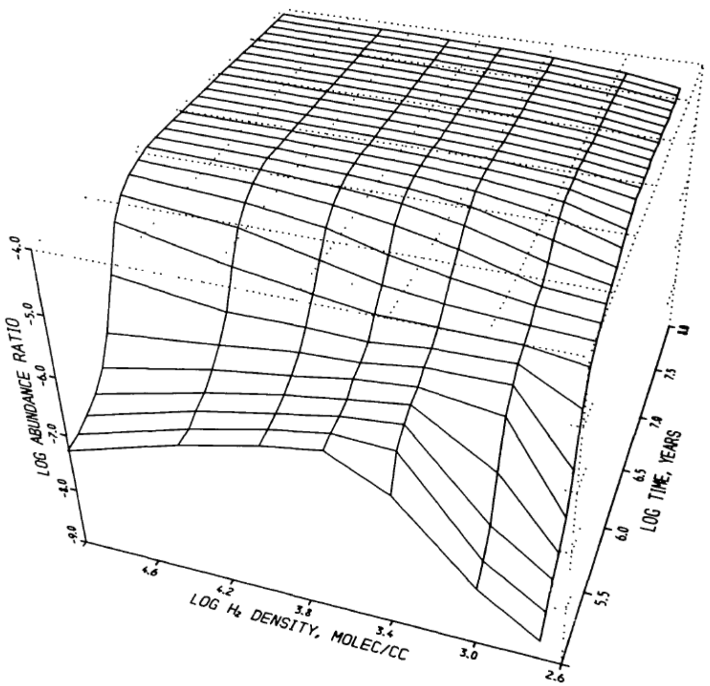
Time-Dependent O_2 Abundance

- Extensive time-dependent calculation carried out by Graedel, Langer, & Frerking (1982)
- For high metal abundance $X(O_2)$ generally < 10^{-7}
- For low metal abundance, $X(O_2)$ can be ~ 10^{-4} for wide rang of H_2 densities as long as clouds have sufficient time for chemistry to approach steady state

O_2 Could Be An Important Species Under Wide Range of Conditions



$n(H_2)$ = 2500 cm^{-3} T = 10 K

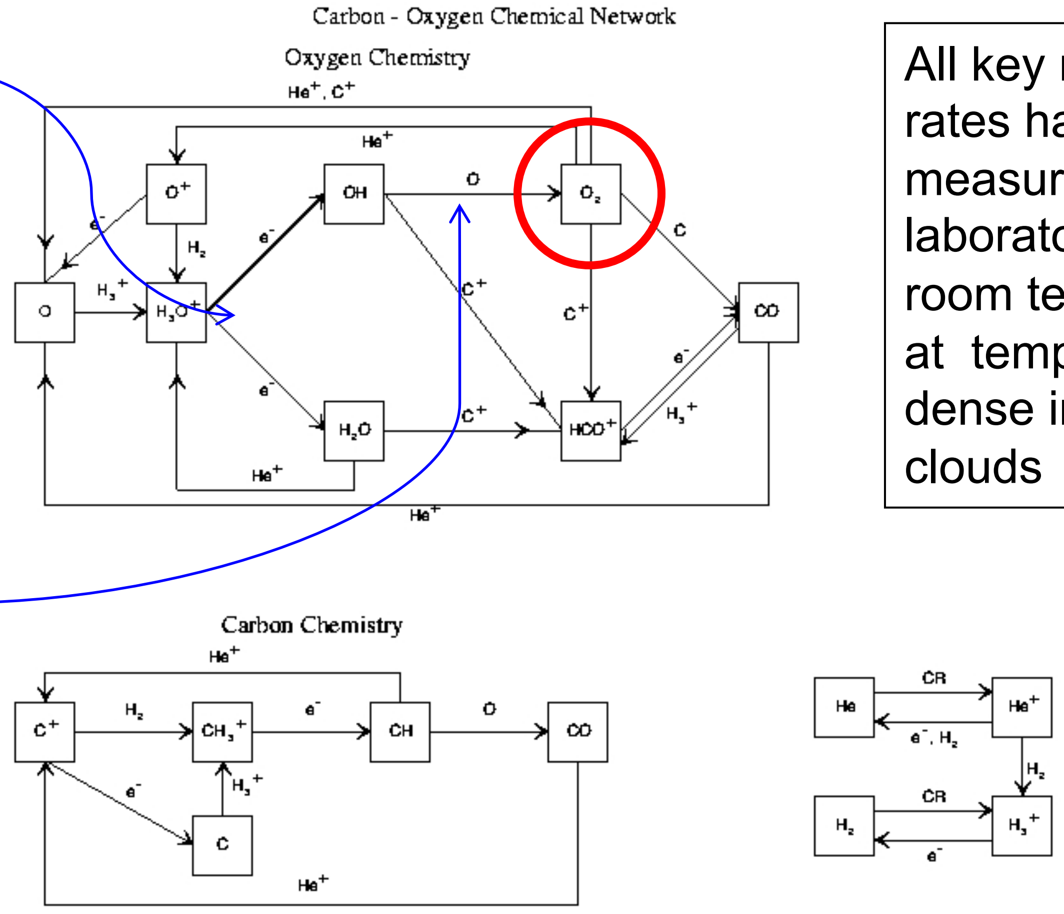


Gas Phase Chemistry for O, H_2O, O_2 and CO is Relatively Simple

Branching ratio measured by ASTRID and CRYRING experiments (Jensen et al. 2000; Neau et al. 2000) $f(H_2O):f(OH) = 0.25:0.75$

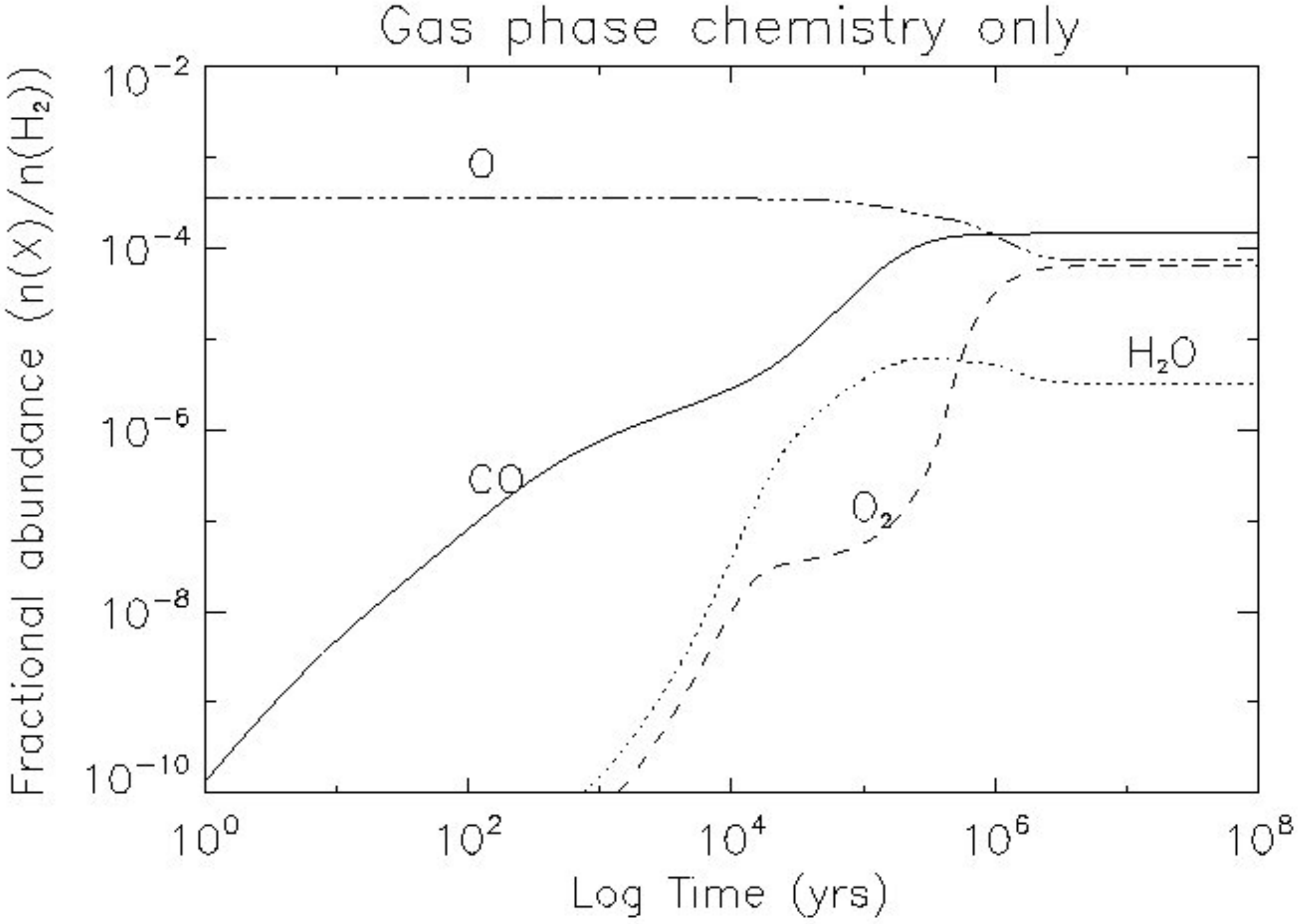
OH + O –> O_2 is an exothermic neutral-neutral reaction

Measurements (Carty et al. (2006) and full quantum calculations (Lique 2010) indicate ~ temp-indep. rate from 300 K to very low temperatures ≅ 4×10^{-11} $cm^3 s^{-1}$



All key reaction rates have been measured in laboratory, both at room temperature & at temperatures of dense interstellar clouds

Standard Gas-Phase Chemistry Models Also Predict Large Abundance of O_2



The time dependent evolution of a gas phase chemistry model. The physical conditions are $n(H_2) = 10^4$ cm^{-3}, T = 10 K, and A_v = 10 mag. The oxygen is initially entirely atomic (K. Willacy).

Searching for O_2 in Interstellar Space

- Terrestrial O_2 makes atmosphere opaque from Earth's surface within frequency range determined by pressure-broadened linewidth
- Two strategies have been utilized to overcome this:
  - Search for $^{16}O^{18}O$
  - Search for extragalactic (red-shifted) O_2

Ground-Based Searches for $^{16}O^{18}O$				
Author(s)	Year	Source(s)	O_2/CO Upper Limits	Comments
Goldsmith+	1985	6 GMCs	0.50 – 4.	
Liszt & Vanden Bout	1985	ρ Oph, Orion	0.13; 0.67	
Combes+	1991	ρ Oph, Orion	0.25; 0.1	
Pagani+	1993	L134N	0.4 - 0.8	Tentative Detection (not confirmed)
Fuente	1993	3 dark clouds	0.15 – 0.29	
Maréchal+	1997	L134N	0.1	Nonconfirmation of Pagani+ (1993)
Liseau+	2010	ρ Oph	0.016	
Pagani+	2017	Orion	-	Line Confusion
Taquet+	2018	IRAS 16293	0.035-0.075	Line Confusion

Ground-Based Searches for Red-Shifted $^{16}O_2$				
Author(s)	Year	Source(s)	O_2/H_2 Upper Limits (10^{-5})	Comments
Liszt	1985	NGC 7674	1.4	8650 km/s
Goldsmith & Young	1989	VII Zw 31	0.4	16280 km/s
Combes	1991	NGC 6240	0.1	7300 km/s
Liszt	1992	NGC 7674	0.14	8700 km/s
Combes & Wiklind	1995	B0218+357	0.14*	$z = 0.685$
Combes+	1997	B0218+357	0.02	$z = 0.685$
Frayer+	1998	5 galaxies	0.31	$0.021 < z < 0.031$

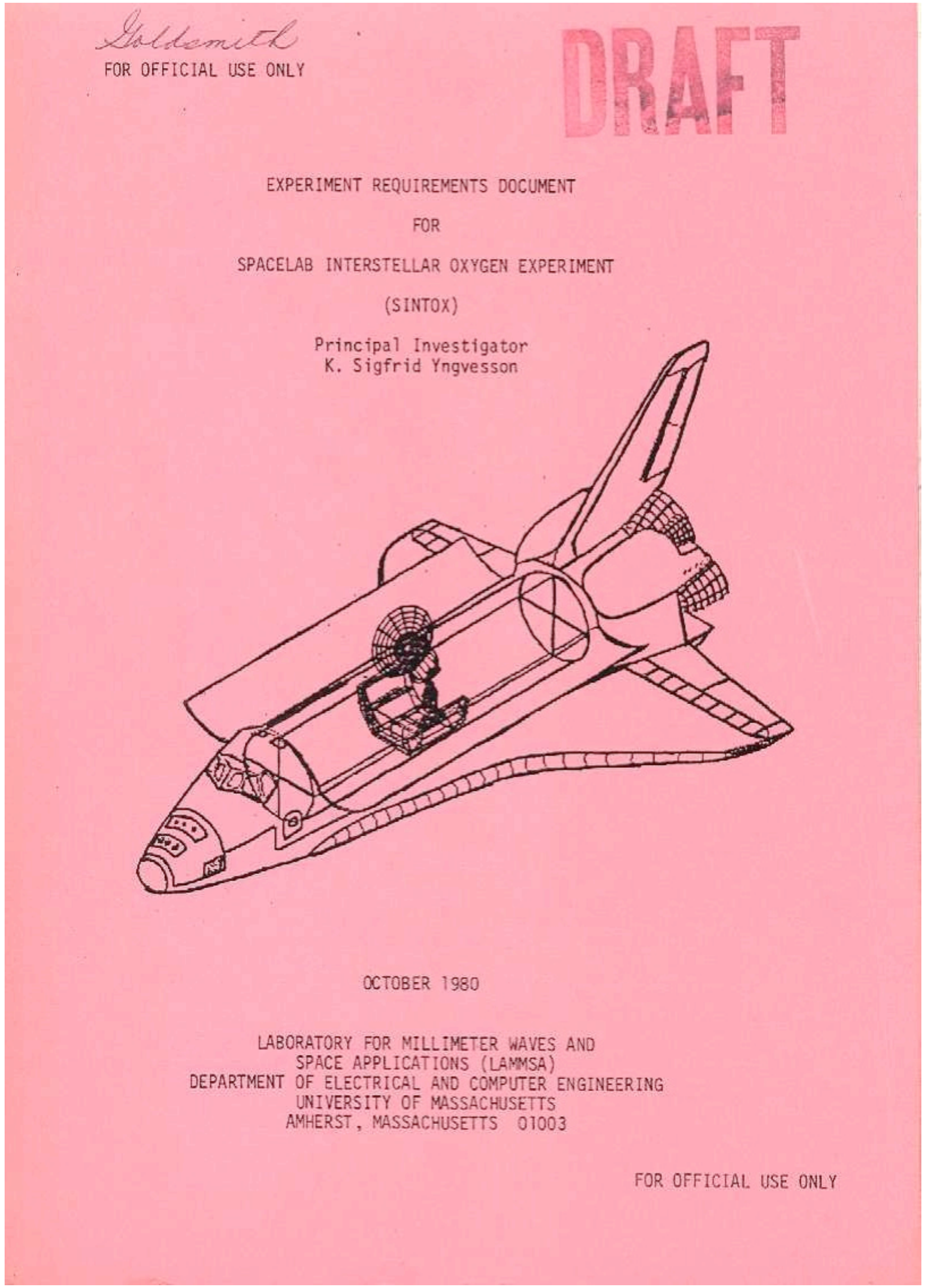
*Assuming $CO/H_2 = 1x10^{-4}$

Searching for O_2 in Molecular Clouds Goes Back a Long Time (1979)

O_2 could be important coolant
O_2 could be a good diagnostic with multiple transitions near 60 GHz

SINTOX experiment proposed for Space Shuttle 3.4m dia. antenna &
500 K (DSB) noise temperature at 60 GHz

Sigfrid Yngvesson was a postdoc in Townes group, working on K-band masers, and then a Professor of Electrical Engineering at the University of Massachusetts, Amherst


Goldsmith

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DRAFT

EXPERIMENT REQUIREMENTS DOCUMENT

FOR

SPACELAB INTERSTELLAR OXYGEN EXPERIMENT

(SINTOX)

Principal Investigator
K. Sigfrid Yngvesson

OCTOBER 1980

LABORATORY FOR MILLIMETER WAVES AND
SPACE APPLICATIONS (LAMMSA)
DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING
UNIVERSITY OF MASSACHUSETTS
AMHERST, MASSACHUSETTS 01003

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Spectroscopy Pathfinder Mission in the Submillimeter – SWAS

Submillimeter Wave Astronomy Satellite

54 x 68cm offset Cassegrain antenna

Passively cooled front end with 2 fixed tuned **Schottky diode 2nd harmonic mixers**

4 Spectral Lines Observed Simultaneously

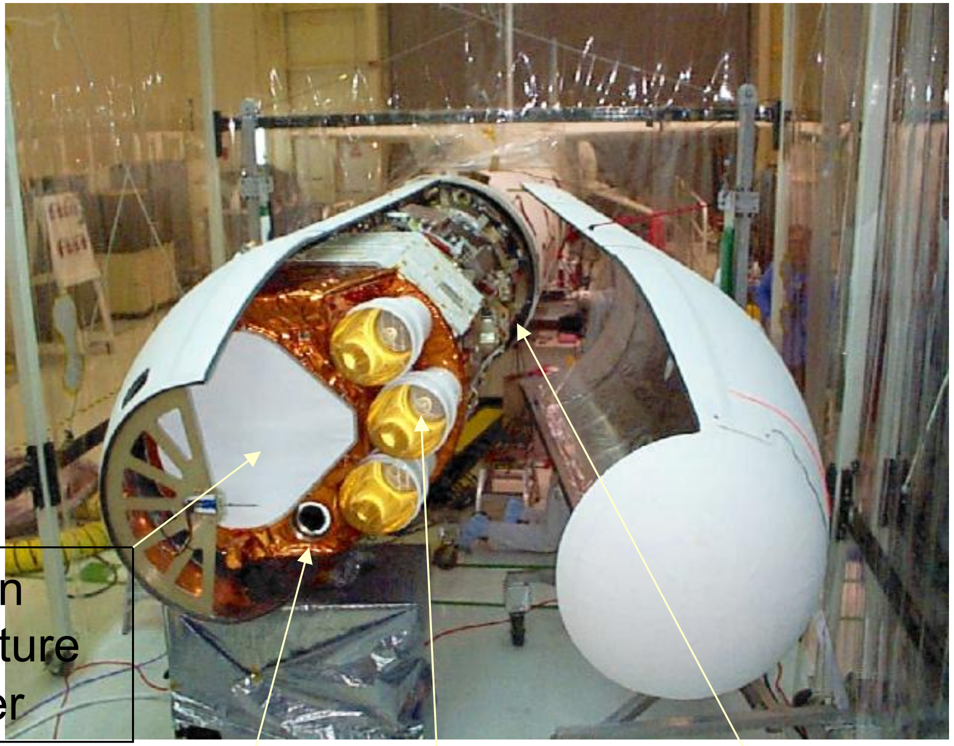
Species	Transition	Frequency	E_u (K)
O_2	**$3_1 - 3_2$**	**487.3 GHz**	**26**
C^0	$^3P_1 - {}^3P_0$	492.1 GHz	24
^{13}CO	5 – 4	550.9 GHz	79
H_2O	$1_{10} - 1_{01}$	556.9 GHz	27

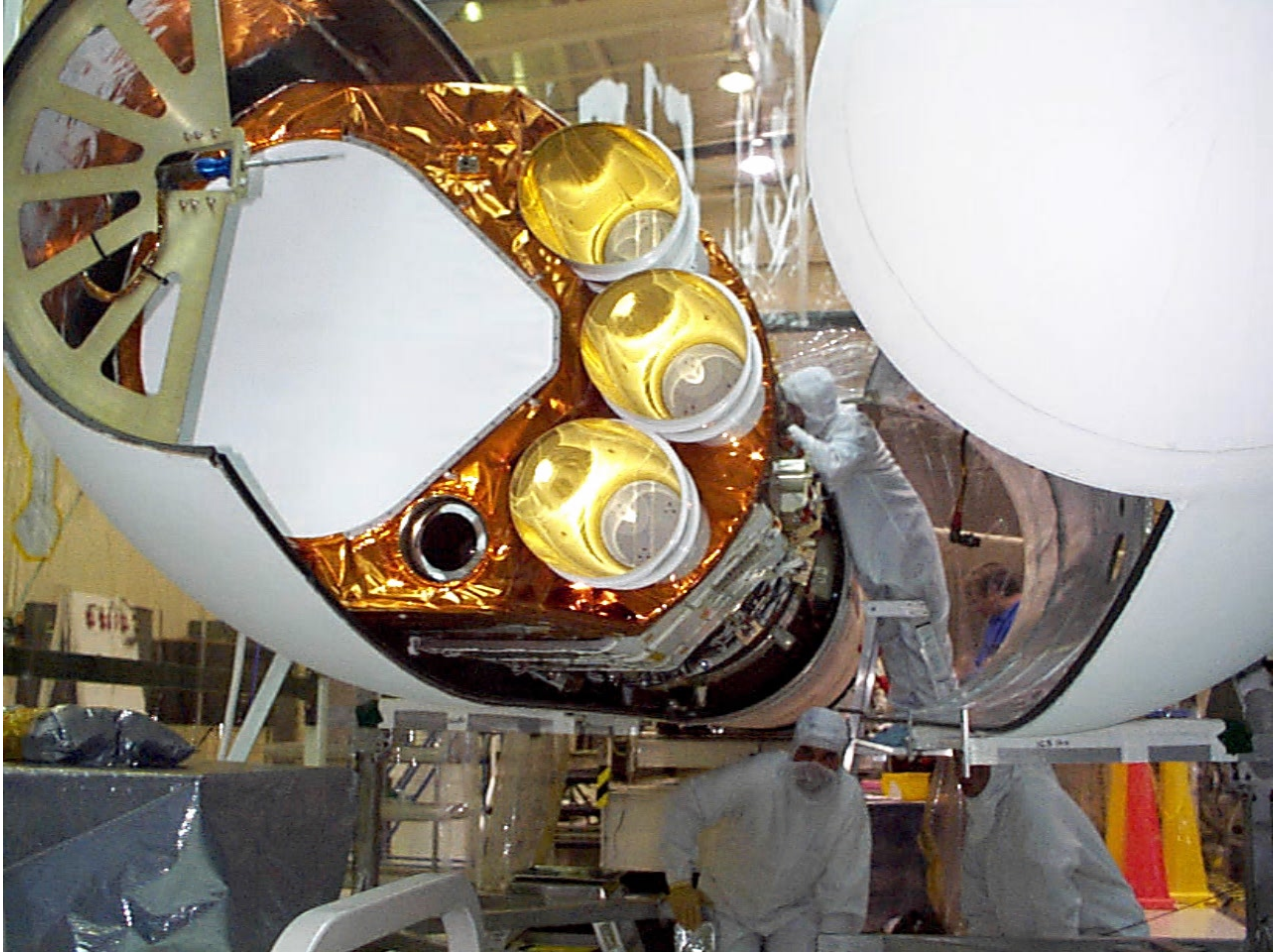
(could retune to the 13CO J = 5-4 line)

Launched 5 Dec 1998

Operated until 21 July 2004

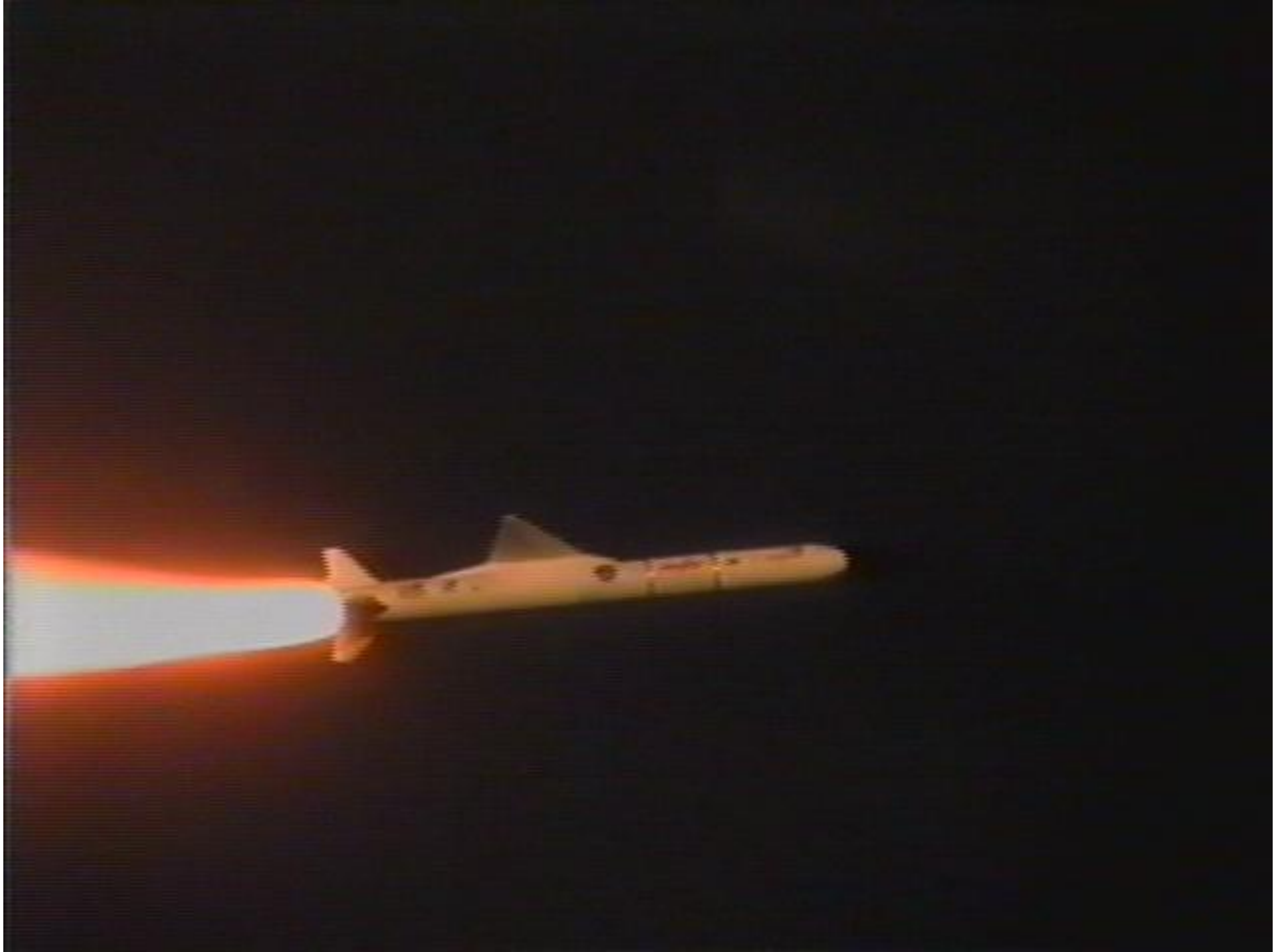
Important results on water & molecular oxygen in dense clouds in interstellar space






December 5, 1998
Vandenberg AFB
Orbital


Orbital

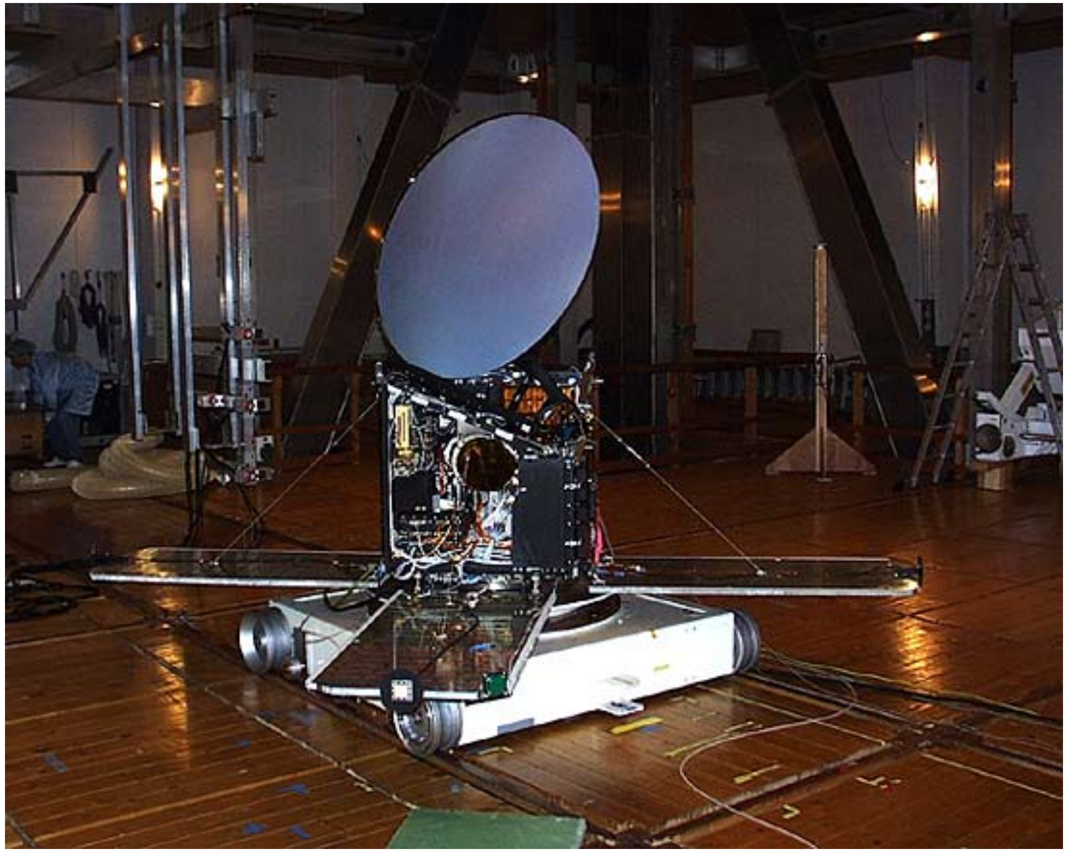


Odin

1.1 m offset Gregorian antenna
Beam size 10' (118 GHz);
2.4'→ 2.1' in submm range
242 kg

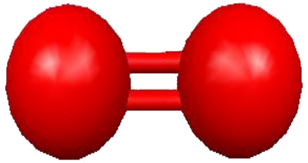
Launched 20 February 2001
Still operating for Earth observations

Multiple receivers:
118 GHz HEMT (O_2)
486- 504 GHz tunable Schottky
541- 581 GHz tunable Schottky
Stirling cycle cooler to 140 K
AOS and digital autocorrelation spectrometers



Sweden + European collaboration

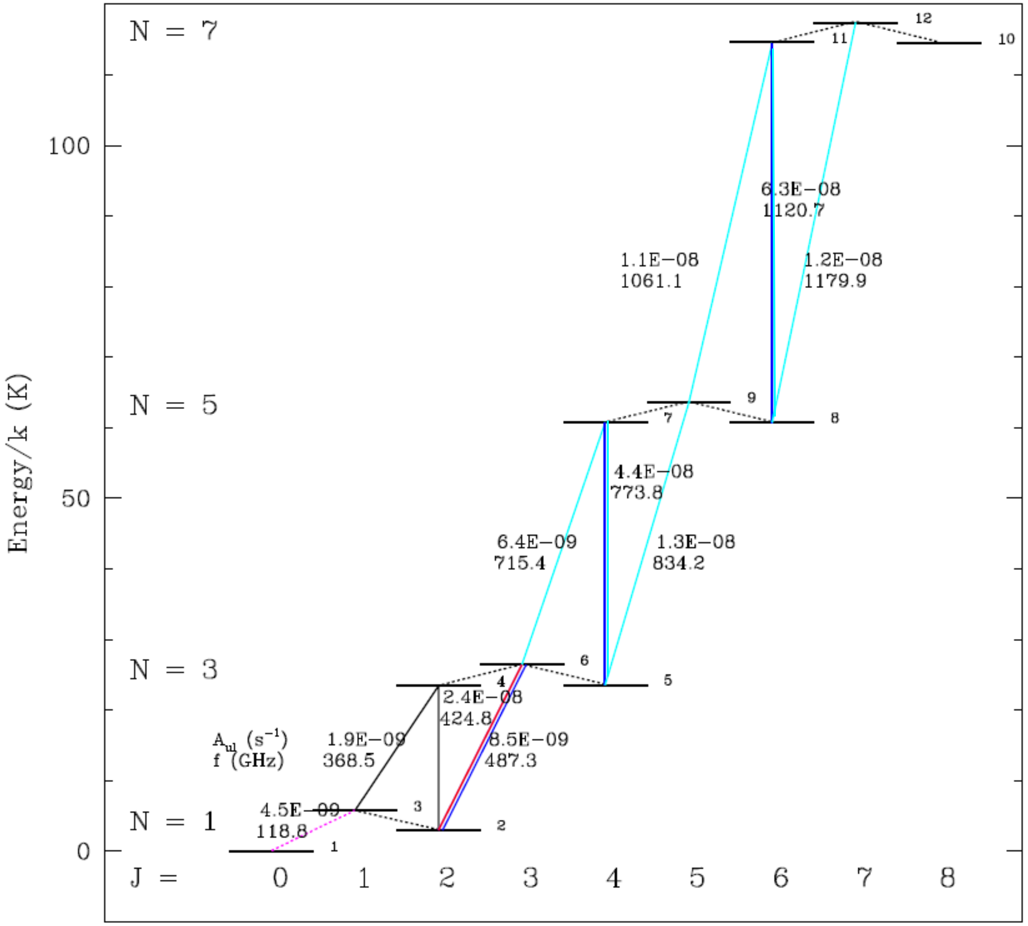
Lower Rotational Levels and Transitions of O_2



O_2 Rotational Levels are Connected by Weak Magnetic Dipole Transitions

Quantum calculations of He-O_2 collisions carried out by Lique (2010) Deex. rate coeffs ≅ $5 \times 10^{-11} cm^3 s^{-1}$

- Critical densities 200 – 1000 cm^{-3}
- Level populations will be in LTE
- Emission will be Optically Thin



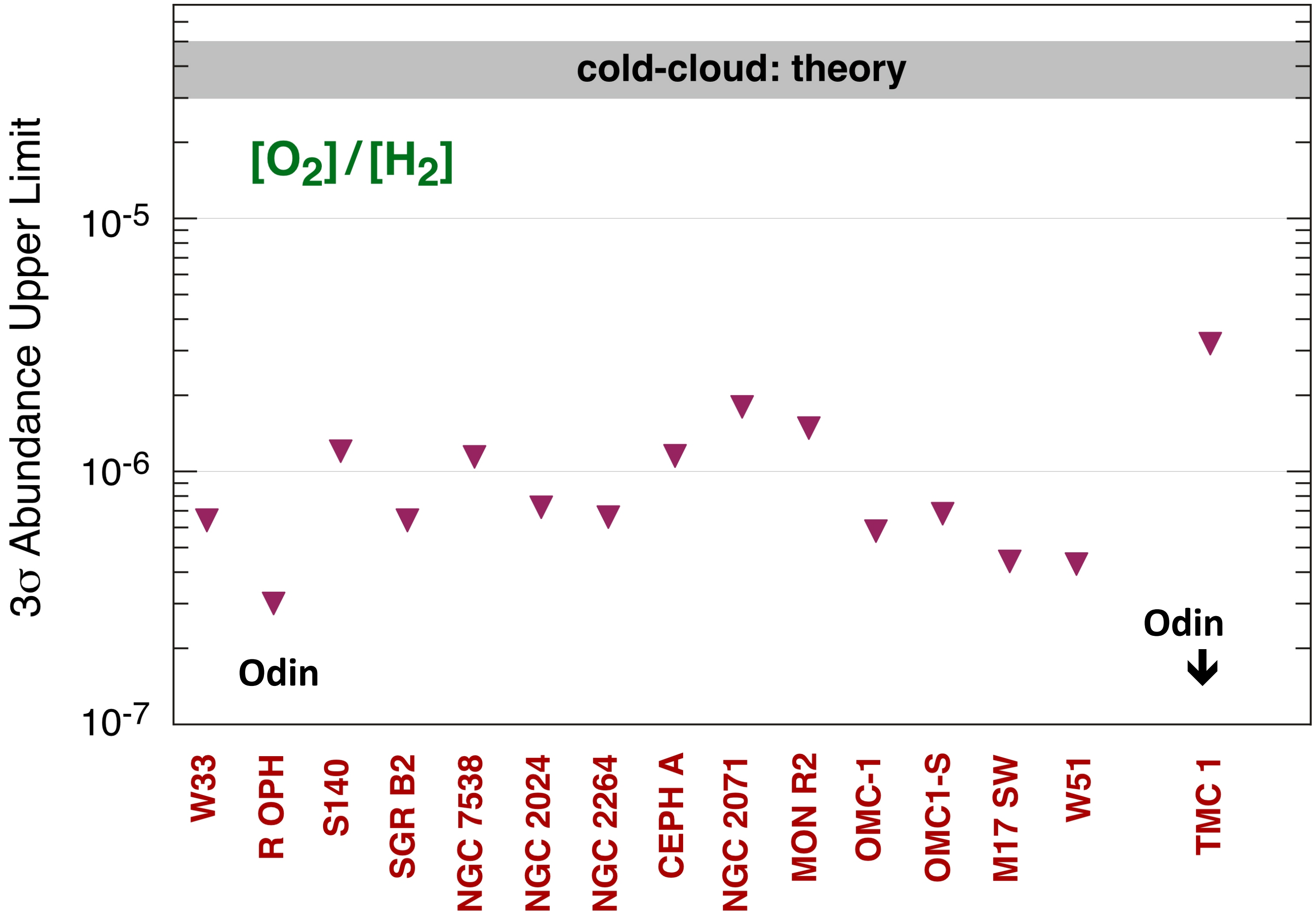
Observed by SWAS

Observed by Odin

Observable with Herschel

Most favorable transitions for Herschel

$X(O_2)$ in IS Clouds from Odin & SWAS is More Than 100X Below that Predicted by Gas-Phase Chemistry



O_2 Results from SWAS & Odin

- No unambiguous detections; one tentative SWAS detection in Rho Oph was probably erroneous
- In 20 clouds, $[O_2]/[H_2] < 10^{-6}$; more than 100x ***below*** prediction of chemical models
- In TMC-1 Odin derived $[O_2]/[H_2] < 2x10^{-7}$
- ***What is going on?***

The “missing piece” is the interstellar dust grains

In early phase of cloud evolution oxygen atoms collide with and stick to dust grains

Result is that gas-phase oxygen abundance is reduced

Available O bound up as CO and little is left to make O_2

Can we Ever Hope to Detect O_2 in Space?

Where might we get oxygen off dust grain mantles and back into gas phase where O_2 can be made?

Two possibilities –

(1) **Interstellar shocks** can "clean" grains and if shock velocity is modest, you get OH formed in postshock gas which then leads to O_2

(2) **Radiation from embedded young stars** heats dust grains to > 100 K, at which point the ice desorbs and water returned to gas phase; this is largely converted to O_2 in ~1 million yr

➔Look at postshock gas and in vicinities of embedded young stars

Herschel Space Observatory

ESA cornerstone mission with major NASA participation

Launched 14 May, 2009

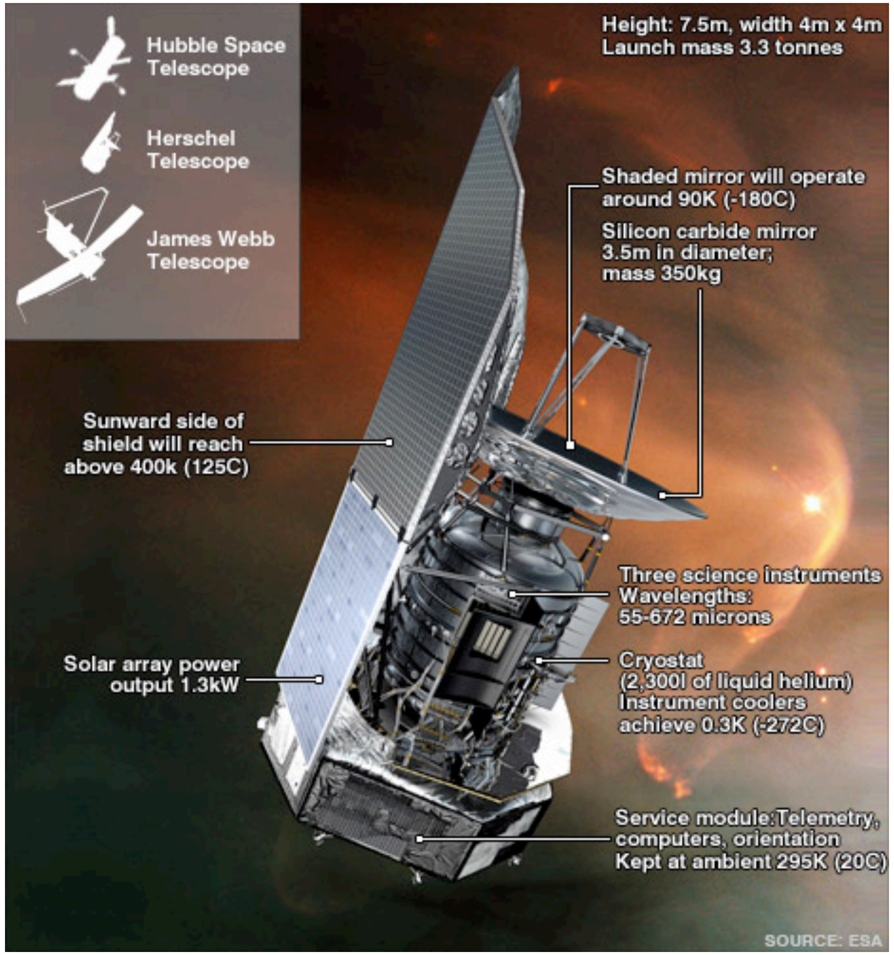
3.5m telescope cooled to~ 80 K

3 instruments including photometers, med.-res. spectrometers and high resolution spectrometer covering 60 µm to 600 µm.

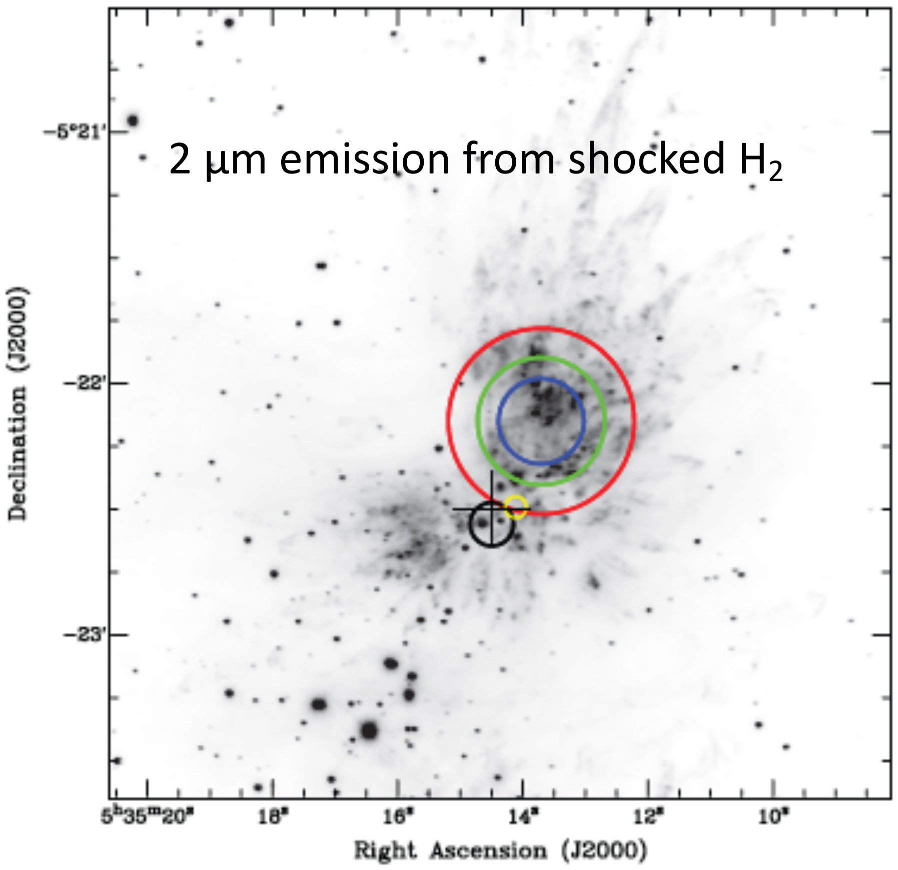
3 prime O_2 lines covered by the HIFI instrument

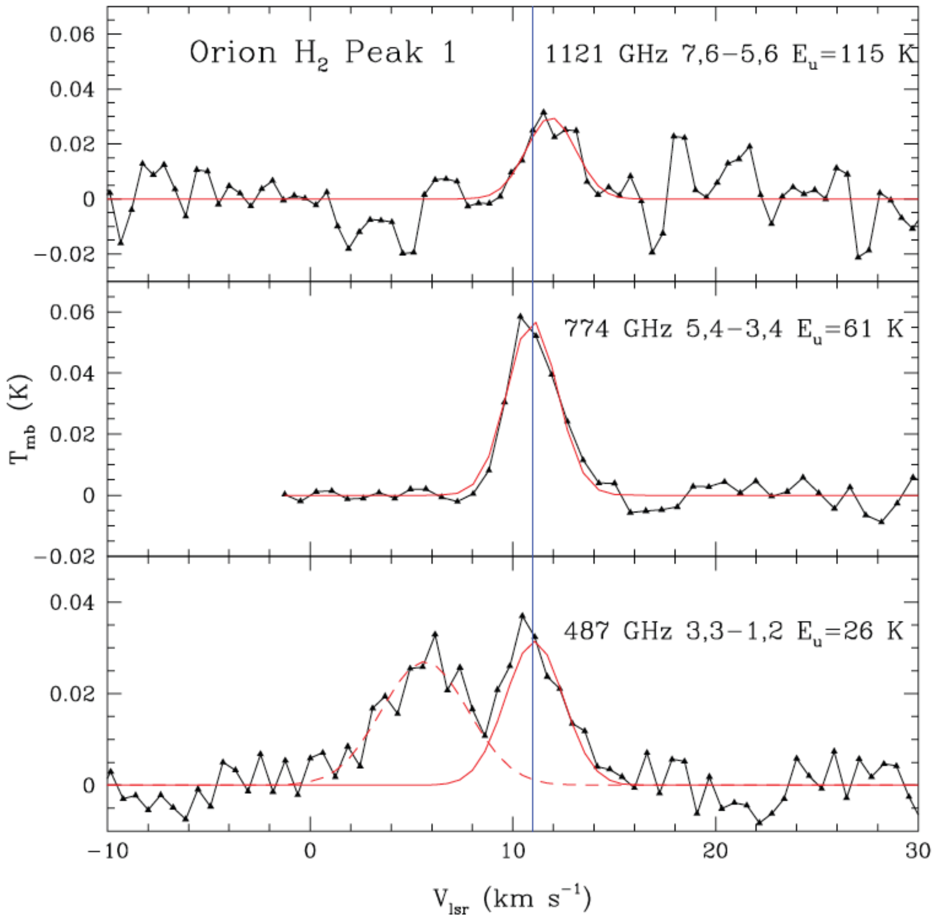
Herschel Oxygen Project ("HOP") targeted 10 most promising sources

Detections **only** in Rho Oph and Orion

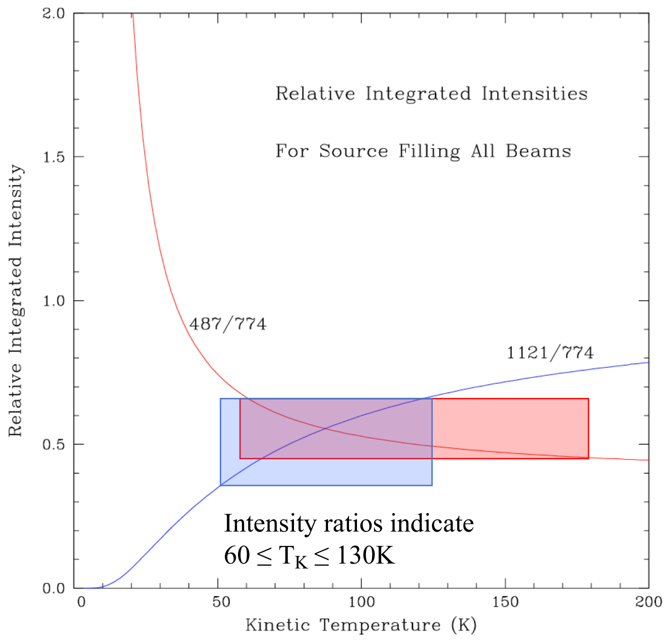


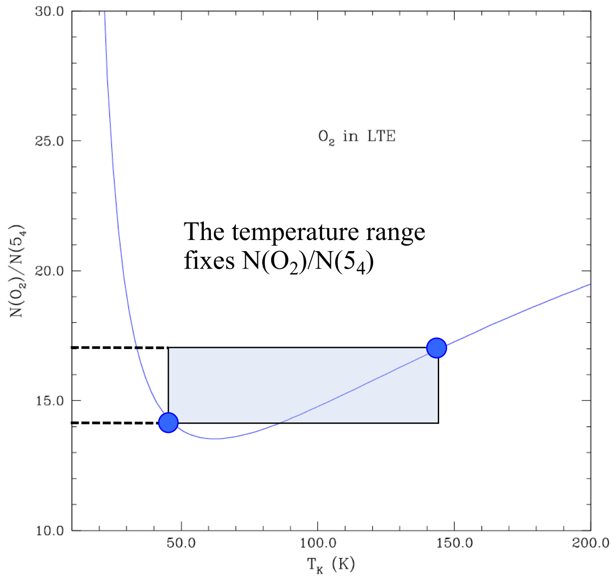
First Multi-Line Detection of O_2: Herschel HIFI Observations of H_2 Peak 1 in Orion





Line Intensity Ratios Determine Kinetic Temperature and Total O_2 Column Density





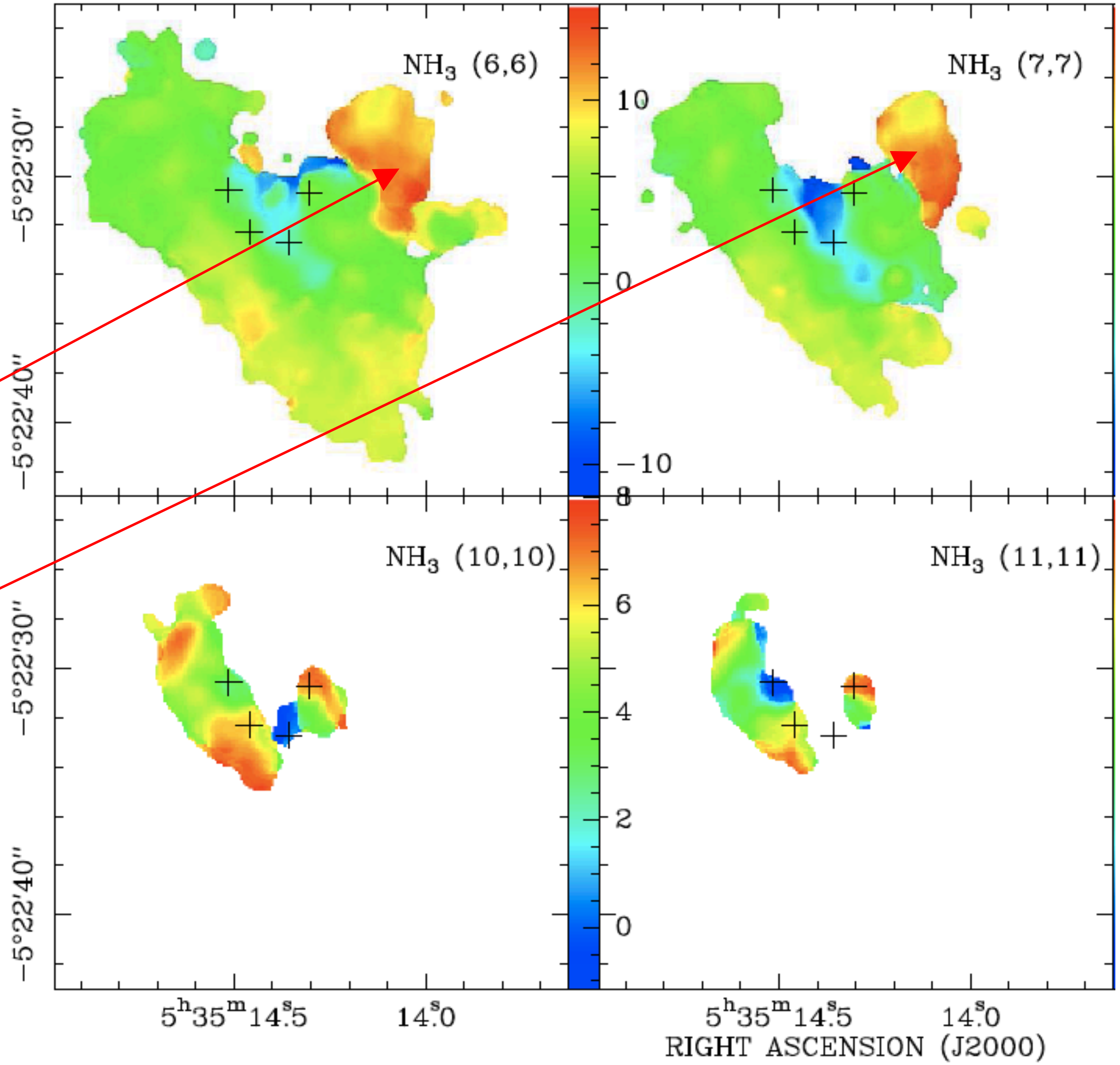
Assuming that the source fills all three Herschel beams:
$N(O_2) = 6.8(+0.7\ -1.0) \times 10^{16}$ cm^{-2} (statistical + kinetic temperature uncertainties)

NH_3 Emission in the Orion Hot Core Region

Moderately excited ammonia inversion lines (Goddi+ 2011)

In one specific region, they have peak at v ~12 km s^{-1} $\alpha = 5^h35^m14.1^s$ δ = -5°22'29''

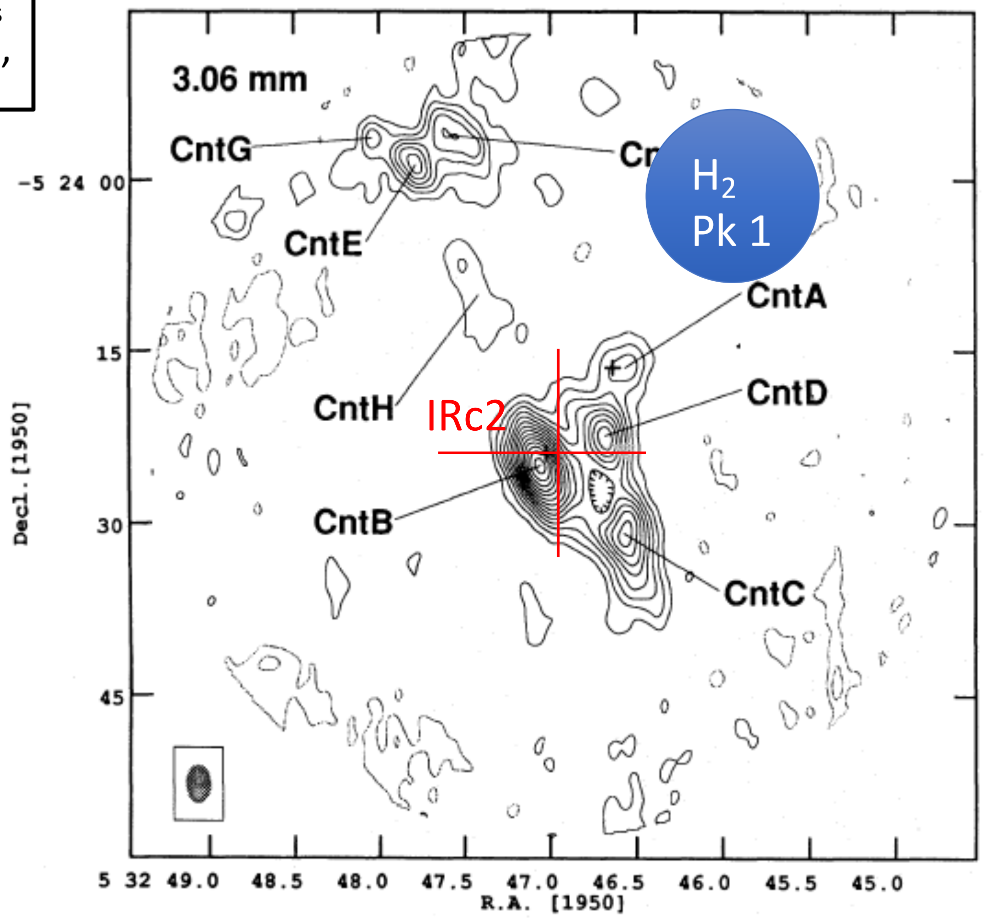
Denoted "Peak A" in earlier ammonia study by Pauls et al. (1983) and in HDO study by Plambeck & Wright (1988)



Where is the Source?

Dust Emission from 3mm Continuum (Murata et al. 1992) is Optically Thin Tracer

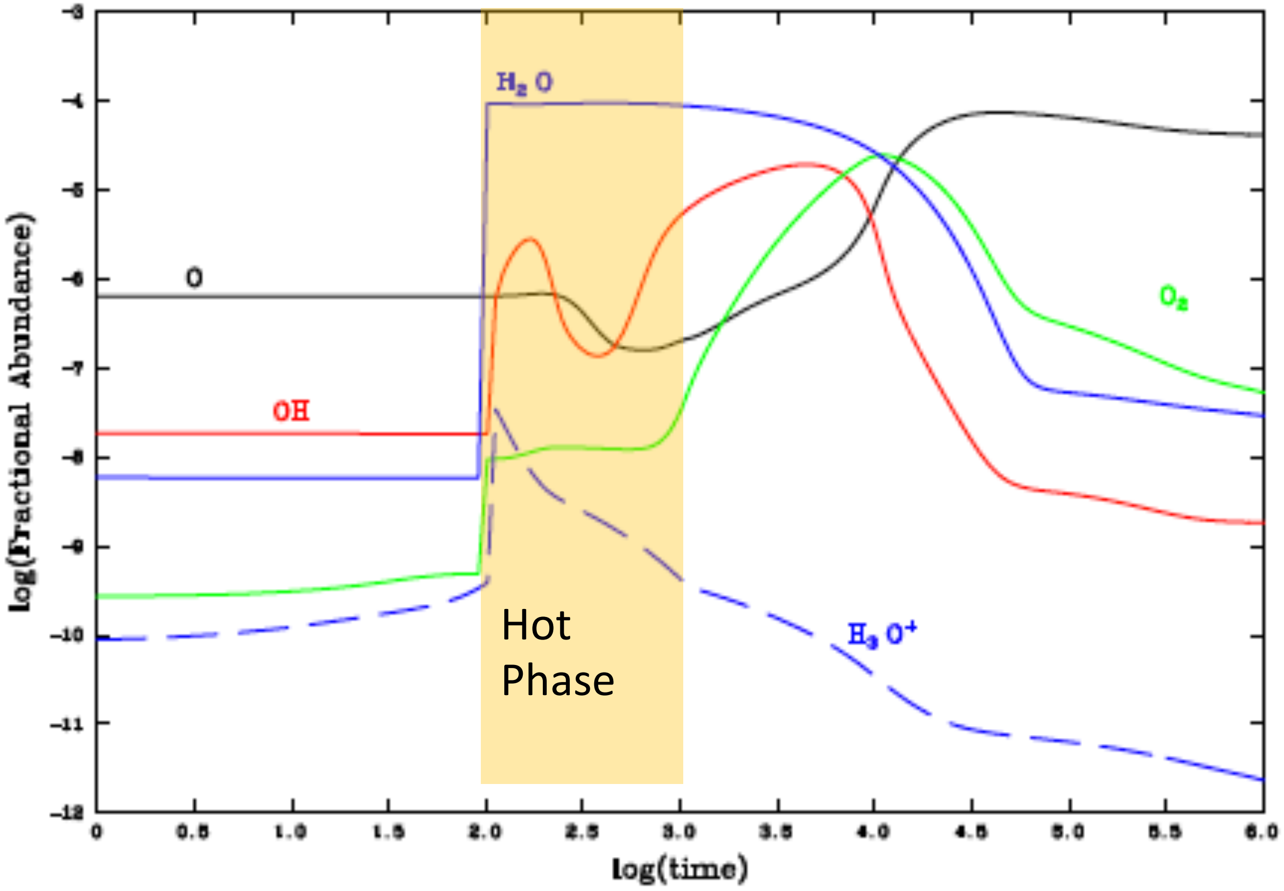
IRc2 (1950)
$\alpha = 5^h32^m47^s$
$\delta = -5^o24'23''$



Cnt D source is coincident with Peak A, Western Clump, and MF4

This is only source with narrow lines & molecular emission in range
$10 < v < 12$ km/s

Low-velocity Shocks are Effective at Producing O_2



12 km/s shock propagating into $n_0(H_2) = 2x10^4\ cm^{-3}$ medium
Modeling by S. Viti (from Chen et al. 2014)

V > 10 km/s gives sufficient heating to allow rapid

$O + H_2$ -> OH + O in **Hot Phase**

Followed by

OH + O -> O_2 + H (exothermic)

V > 15 km/s produces high enough T to allow **back reaction**

O_2 + H -> OH + H
~exp(-8750/T)

Pros and Cons of Shock Model for O_2 Abundance Enhancement

- Shock model can produce up to $X(O_2)$ = few $x10^{-5}$ for 10^3-$3x10^4$ yr after shock passage with V_{shock} = 10 – 15 km s^{-1}
- Line profile is a question, as one would expect velocity shifts, although this could be avoided if shock lies in plane of the sky
- Need to get substantial O in gas BEFORE the shock. This could come from higher-velocity J-type shocks in vicinity as indicated by H_2 emission, by sputtering, or by UV from PDR surface
- Source size and location are still unclear: Chen et al. (2014) with observations of Peak A show source actually closer to H_2 Peak 1 and that source is small, implying that peak column density ~ 10^{18} cm^{-2}
- O_2 velocity agrees with that of H_2O masers in the vicinity. Shock in plane of sky => maximum maser gain along LOS

O_2 in ρ Oph A SM1

Color is integrated O_2 intensity

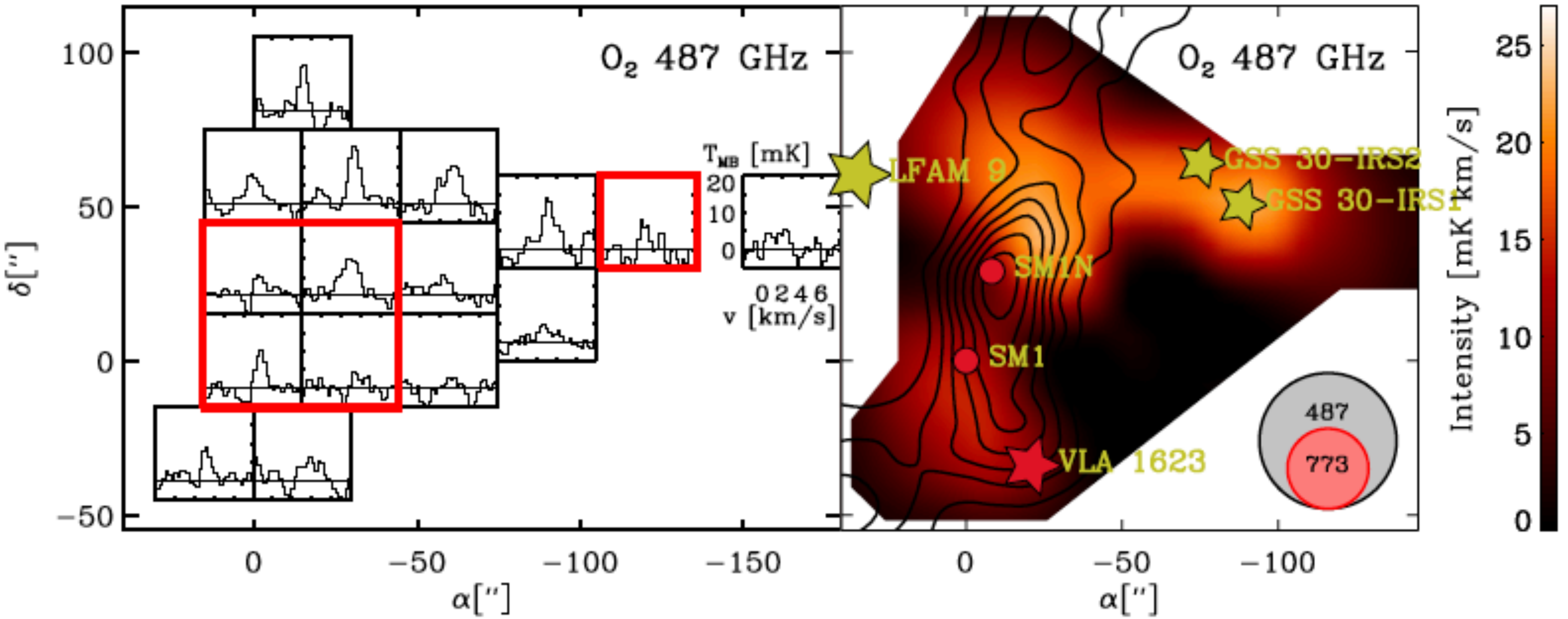


Fig. 3. *Left*: map of ρ Oph A in the O_2 $(3_3–1_2)$ 487 GHz line with HIFI. At the positions of the red frames oversampled O_2 $(5_4–3_4)$ 773 GHz spectra were obtained. Scales in km s^{-1} and mK are indicated in the spectrum of the off-position (westernmost frame). *Right*: contour-colour map of the data shown in *the left panel*. The colour bar for the integrated intensity in mK km s^{-1} is shown to the *right*. The contours outline integrated N_2H^+ (3–2) emission.

Larsson & Liseau 2017; see also Liseau et al. 2012

O_2 in ρ Oph A SM1

- Total of 38.5 h on 487 GHz line and 8.5 h on 773 GHz line with Herschel HIFI resulted in uniquely sensitive observations
- Extended source & weak O_2 emission => “modest” O_2 fractional abundance, $X(O_2) = 5x10^{-8}$
- $X(O_2)/X(H_2O)$ ~ 10 [Huge!]
- Complex source geometry and locations of luminous sources are a challenge for modeling
  - The role of outflows, shocks, grain-surfaces, and gas-phase chemistry are all unclear
  - The observed gas-phase O_2 abundance may be relatively transient; O_2 enhancement likely to be followed by depletion onto grain surface, but this is not certain

Where Do Things Stand and What is Next?

OBSERVATIONS

- Gas-phase O_2 fractional abundance is low, a very small fraction of available oxygen, even with detections in relatively quiescent regions such as ρ Oph A where $X(O_2) = 5\times10^{-8}$.
- Abundance in postshock gas (plausible explanation for Orion) is likely significantly higher (~10^{-5})
- Is oxygen atom depletion onto grain surfaces responsible?
- Future space observations are far off; ground-based observations can be pursued

THEORY & MODELING

- Increased binding energy of oxygen atoms on grain surfaces (~1700 K as compared to previous estimate of ~800 K; He et al. 2015) contributes to low gas-phase O_2 abundance
- An interesting question is the possible connection between interstellar O_2 and that found in comets (Taquet et al. 2016, 2018)
- Some of the questions relating to photodissociation are connected to the abundance of abiotic molecular oxygen in exoplanet atmospheres (Tian et al. 2014)